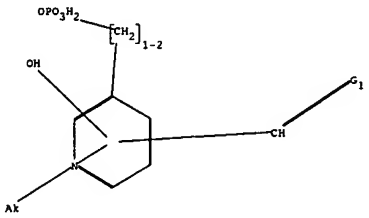
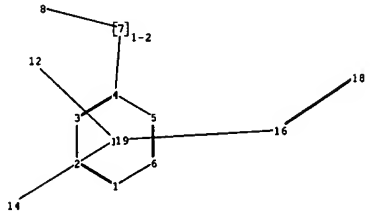
C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\nbvfghj.str



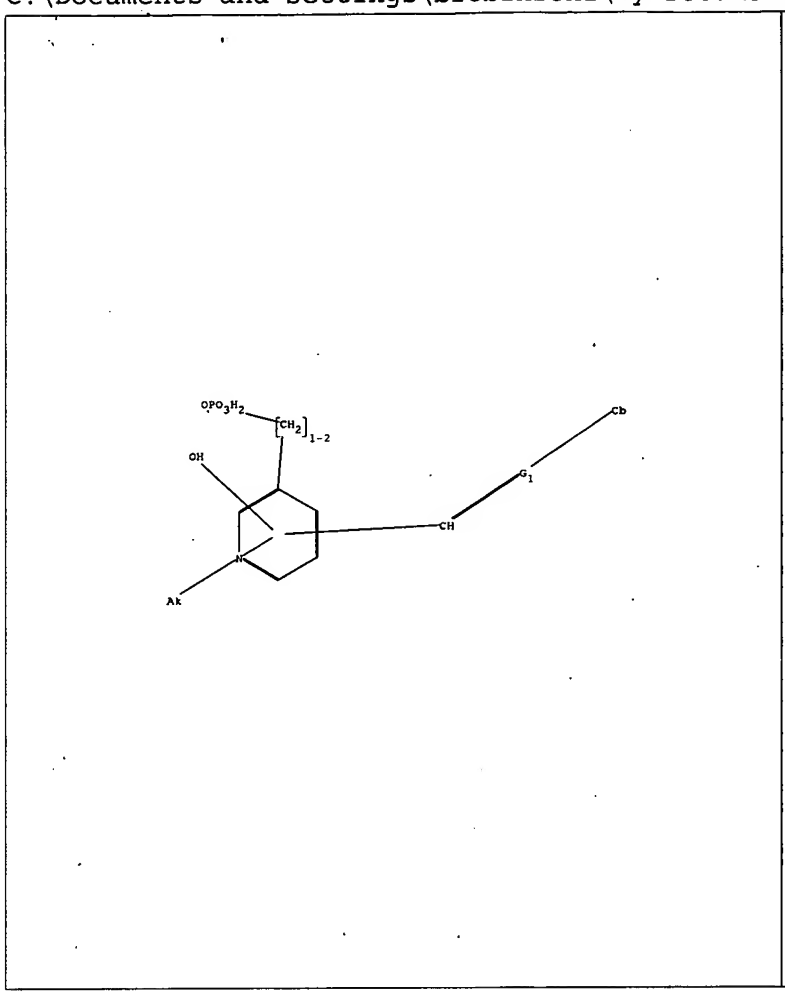


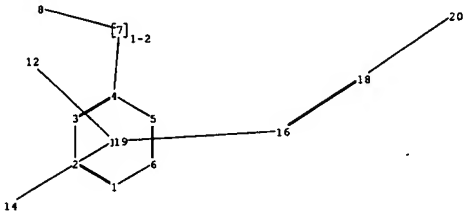
chain nodes :
7 8 12 14 16 18
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 7-8 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
16-18
exact bonds :
4-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:Atom
14:CLASS 15:Atom 16:CLASS 18:CLASS 19:Atom

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\vnjgm.str





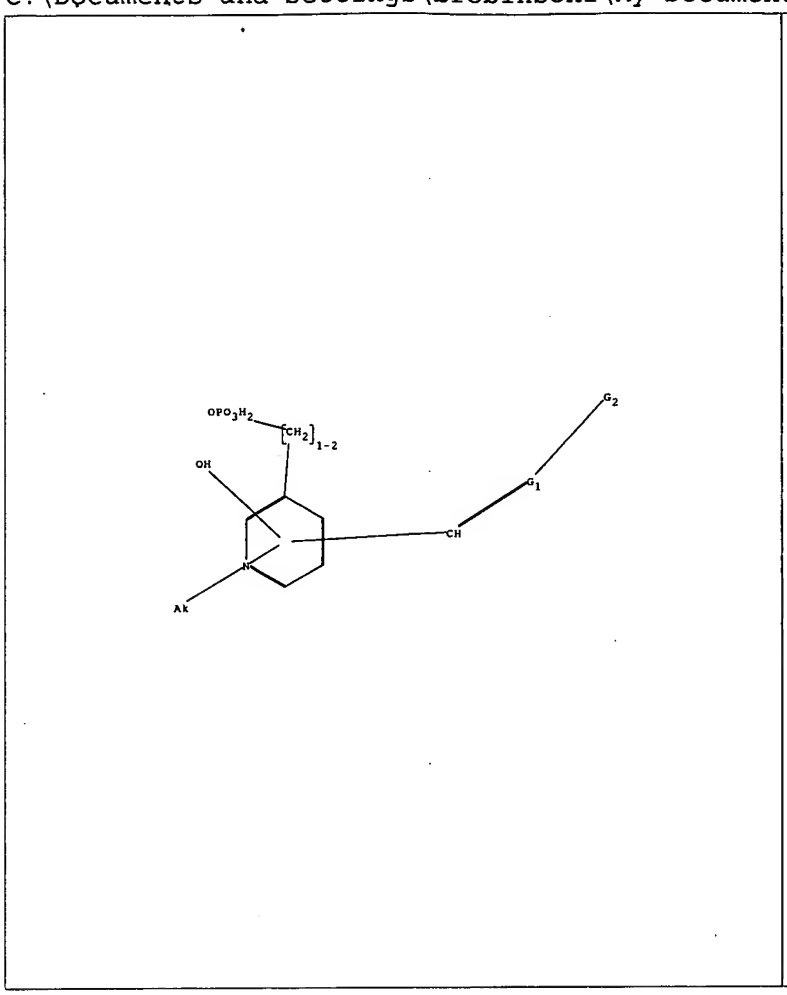
chain nodes :
7 8 12 14 16 18 20
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 7-8 16-18 18-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
16-18 18-20
exact bonds :
4-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

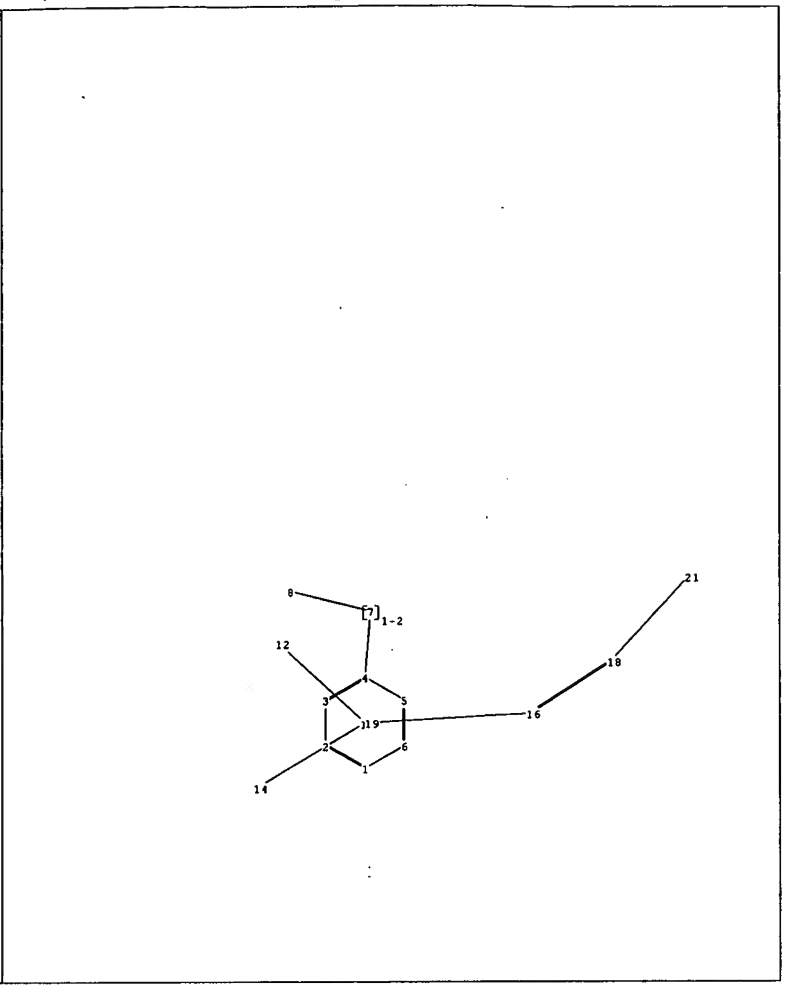
G1:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:Atom
14:CLASS 15:Atom 16:CLASS 18:CLASS 19:Atom 20:Atom
Generic attributes :
20:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

Type of Ring System : Polycyclic

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\anghuty.str





chain nodes :
7 8 12 14 16 18 21
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 7-8 16-18 18-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
16-18 18-21
exact bonds :
4-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:C,N

G2:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:Atom
14:CLASS 15:Atom 16:CLASS 18:CLASS 19:Atom 21:CLASS

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

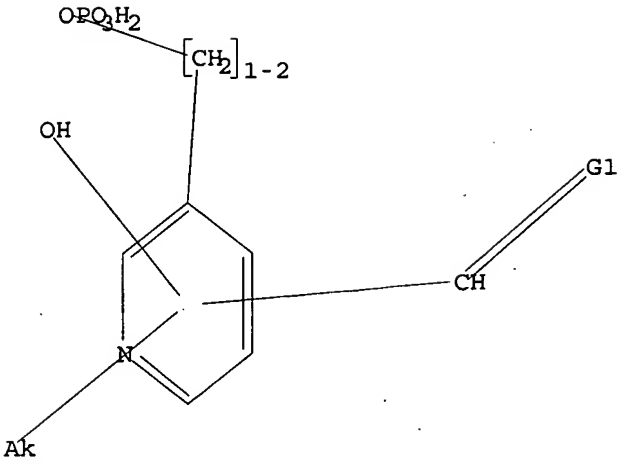
NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

Updated Search

```
 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN     Welcome Banner and News Items
 NEWS IPC8      For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:10:20 ON 25 JAN 2008

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 13:10:25 ON 25 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   24 JAN 2008  HIGHEST RN 1000773-19-2
DICTIONARY FILE UPDATES:  24 JAN 2008  HIGHEST RN 1000773-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My
Documents\stnweb\Queries\nbvfghj.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
```

Updated Search



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 13:12:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      150 TO ITERATE

100.0% PROCESSED      150 ITERATIONS                          23 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2266 TO     3734
PROJECTED ANSWERS:             173 TO      747

L2            23 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:13:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     3147 TO ITERATE

100.0% PROCESSED     3147 ITERATIONS                         358 ANSWERS
SEARCH TIME: 00.00.01

L3           358 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                           179.74     179.95

FILE 'HCAPLUS' ENTERED AT 13:13:06 ON 25 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```


Updated Search

held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 25 Jan 2008 VOL 148 ISS 5
FILE LAST UPDATED: 24 Jan 2008 (20080124/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 343 L3

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.69	182.64

FILE 'REGISTRY' ENTERED AT 13:13:12 ON 25 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JAN 2008 HIGHEST RN 1000773-19-2
DICTIONARY FILE UPDATES: 24 JAN 2008 HIGHEST RN 1000773-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

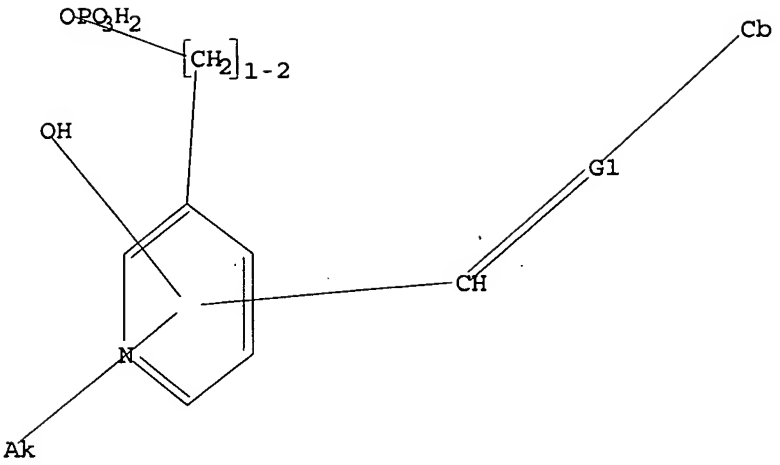
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\vnjgm.str

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR

Updated Search



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 13:14:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 150 TO ITERATE

100.0% PROCESSED 150 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2266 TO 3734
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:14:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3152 TO ITERATE

100.0% PROCESSED 3152 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L7 0 SEA SSS FUL L5

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\anghuty.str

L8 STRUCTURE UPLOADED

=> s l8
SAMPLE SEARCH INITIATED 13:15:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 150 TO ITERATE

100.0% PROCESSED 150 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.01

Updated Search

```
FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:          2266 TO     3734
PROJECTED ANSWERS:              119 TO      641

L9            19 SEA SSS SAM L8

=> s l8 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:15:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      3147 TO ITERATE

100.0% PROCESSED      3147 ITERATIONS                                266 ANSWERS
SEARCH TIME: 00.00.01

L10           266 SEA SSS FUL L8

=> file hcaplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     357.64     540.28

FILE 'HCAPLUS' ENTERED AT 13:15:35 ON 25 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 25 Jan 2008  VOL 148 ISS 5
FILE LAST UPDATED: 24 Jan 2008  (20080124/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l10
L11           210 L10

=> s l11 and pd < may 2002
      22700568 PD < MAY 2002
                 (PD<20020500)
L12           197 L11 AND PD < MAY 2002

=> d l12, ibib abs fhitstr, 1-10

L12  ANSWER 1 OF 197  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2003:833703  HCAPLUS
DOCUMENT NUMBER:          141:19546


Updated Search
```

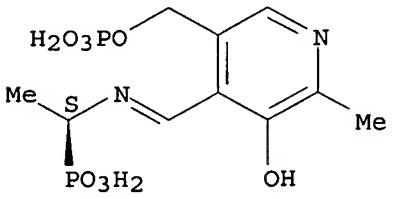
TITLE: A single anion binding site helps define the reaction mechanism of alanine racemase
AUTHOR(S): Stamper, Geoffrey F.; Ringe, Dagmar
CORPORATE SOURCE: Program in Biophysics, Brandeis University, Waltham, MA, 02454, USA
SOURCE: ACA Transactions (2001), Volume Date 2000, 35(Using Crystallography to Understand Enzyme Mechanism), 1-8
CODEN: ATCRCS
PUBLISHER: American Crystallographic Association
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Alanine racemase is a pyridoxal 5'-phosphate dependent enzyme that catalyzes the isomerization of the amino acid alanine. The anabolic function of the enzyme in bacteria is to provide the D-alanine required for cell wall biosynthesis. Though the enzyme has long been studied as an antibacterial target, recent studies have focused on understanding the details of the reaction mechanism. Since the enzyme recognizes both isomers of the substrate, the question has long been asked whether there is one base that can abstract the alpha proton from either isomer of the substrate or whether there are two bases, one on each side of the substrate PLP complex. Structural evidence indicates that the active site Lys39 is in position to act as a base for proton abstraction from the D-isomer of the alanine substrate and Tyr265' is in position to act as a base for the L-isomer. This implies that each base is specific for Cα proton abstraction from a particular isomer of the alanine substrate. In support of the proposed mechanism, we report here addnl. structural evidence that shows there is a single phosphonate binding site, regardless of stereochem. If this phosphonate is representative of the binding of substrate, then there is only a single binding mode for the substrate, and two bases, Lys39 and Tyr265', are required for catalysis.

IT 228560-70-1D, complexes with alanine racemase
RL: PRP (Properties)
(crystal structure; crystallog. study indicates that a single anion binding site helps define the reaction mechanism of alanine racemase)

RN 228560-70-1 HCAPLUS
CN Phosphonic acid, [(1S)-1-[[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



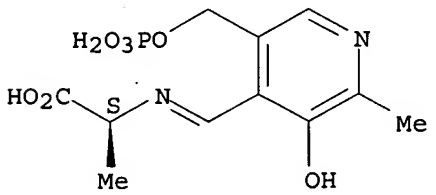
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:414278 HCAPLUS
DOCUMENT NUMBER: 137:151746
TITLE: Reaction mechanism of alanine racemase from Bacillus stearothermophilus: X-ray crystallographic studies of the enzyme bound with N-(5'-phosphopyridoxyl)alanine
AUTHOR(S): Watanabe, Akira; Yoshimura, Tohru; Mikami, Bunzo;

Updated Search

Hayashi, Hideyuki; Kagamiyama, Hiroyuki; Esaki, Nobuyoshi
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan
SOURCE: Journal of Biological Chemistry (2002), 277(21), 19166-19172
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystal structures of alanine racemase bound with reaction intermediate analogs, N-(5'-phosphopyridoxyl)-L-alanine (PLP-L-Ala) and N-(5'-phosphopyridoxyl)-D-alanine (PLP-D-Ala), were determined at 2.0-Å resolution with the crystallog. R factor of 17.2 for PLP-L-Ala and 16.9 for PLP-D-Ala complexes. They were quite similar not only to each other but also to the structure of the native pyridoxal 5'-phosphate (PLP)-form enzyme; root mean square deviations at Cα among the three structures were less than 0.28 Å. The side chains of the amino acid residues around the PLP-L-Ala and PLP-D-Ala were virtually superimposable on each other as well as on those around PLP of the native holoenzyme. The α-hydrogen of the alanine moiety of PLP-L-Ala was located near the OH of Tyr265', whereas that of PLP-D-Ala was near the NZ of Lys39. These support the previous findings that Tyr265' and Lys39 are the catalytic bases removing α-hydrogen from L- and D-alanine, resp. The prerequisite for this two-base mechanism is that the α-proton abstracted from the substrate is transferred (directly or indirectly) between the NZ of Lys39 and the OH of Tyr265'; otherwise the enzyme reaction stops after a single turnover. Only the carboxylate oxygen atom of either PLP-Ala enantiomer occurred at a reasonable position that can mediate the proton transfer; neither the amino acid side chains nor the water mols. were located in the vicinity. Therefore, we propose a mechanism of alanine racemase reaction in which the substrate carboxyl group directly participates in the catalysis by mediating the proton transfer between the two catalytic bases, Lys39 and Tyr265. The results of MO calcn. also support this mechanism.
IT 61652-32-2D, complex with alanine racemase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(crystal structure of Bacillus stearothermophilus alanine racemase bound with N-(5'-phosphopyridoxyl)alanine)
RN 61652-32-2 HCAPLUS
CN L-Alanine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

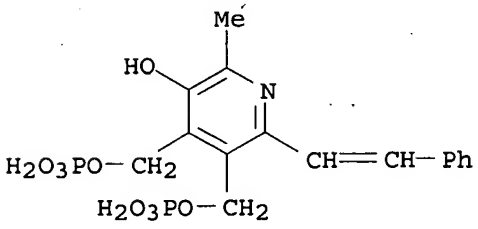
L12 ANSWER 3 OF 197 HCAPLUS

Updated Search

ACCESSION NUMBER: 2001:812441 HCAPLUS
DOCUMENT NUMBER: 136:112222
TITLE: Actions of a series of PPADS analogs at P2X1 and P2X3 receptors
AUTHOR(S): Brown, Sean G.; Kim, Yong-Chul; Kim, Soon-Ai; Jacobson, Kenneth A.; Burnstock, Geoffrey; King, Brian F.
CORPORATE SOURCE: Autonomic Neuroscience Institute, Royal Free and University College Medical School, London, NW3 2PF, UK
SOURCE: Drug Development Research (2001), 53(4), 281-291
CODEN: DDREDK; ISSN: 0272-4391
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Seven PPADS (Pyridoxal-5'-Phosphate 6-Azophenyl 2',4'-DiSulfonate) analogs were investigated at Group 1 P2X receptors expressed in Xenopus oocytes. All seven analogs potently inhibited P2X1 (IC50 range, 5-32 nM) and P2X3 (IC50 range, 22-345 nM), the two Group I P2X receptor subtypes. Analogs showed greater inhibitory activity where the pyridoxal moiety of PPADS contained a 5'-phosphonate group, rather than a 5'-phosphate group. Analogs also showed greater potency where disulfonate groups were removed from, or substituted at, the azophenyl moiety. The most active analog was MRS 2257 (pyridoxal-5'-phosphonate 6-azophenyl 3',5'-bismethylenephosphonate) at P2X1 (IC50, 5 nM) and P2X3 (IC50, 22 nM) receptors, being 14-fold and 10-fold more potent than PPADS itself. MRS 2257 produced a non-surmountable inhibition when tested against a range of ATP concns., although blockade was reversed by about 85% after 20 min of washout. TNP-ATP and Ip5I were equipotent with MRS 2257 at P2X1 receptors, whereas TNP-ATP was 64-fold more potent than MRS 2257 at P2X3 receptors. In conclusion, the PPADS template can be altered at the pyridoxal and Ph moieties to produce P2X1 and P2X3 receptor antagonists showing higher potency and greater degree of reversibility than the parent compound at these Group I P2X receptors.

IT 390818-02-7, MRS 2259
RL: PAC (Pharmacological activity); BIOL (Biological study)
(structure activity relationships of PPADS analogs as P2X1 and P2X3 receptor antagonists)
RN 390818-02-7 HCAPLUS
CN 3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-2-(2-phenylethenyl)-, α,α'-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:130228 HCAPLUS
DOCUMENT NUMBER: 134:310075
TITLE: Effect of phosphate on stability of pyridoxal in the presence of lysine

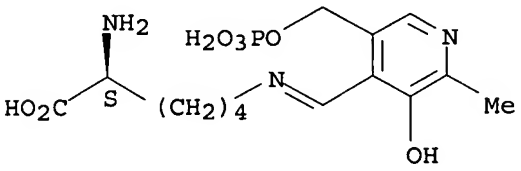
Updated Search

AUTHOR(S): Huang, Tzou-Chi; Chen, Ming-Hung; Ho, Chi-Tang
CORPORATE SOURCE: Department of Food Science, National Pingtung University of Science and Technology, Pingtung, 912, Taiwan
SOURCE: Journal of Agricultural and Food Chemistry (2001), 49(3), 1559-1563
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stability of vitamin B6 in aqueous solution was investigated. Schiff base formation is the major reaction between the ε-amino group of lysine and the aldehyde group of both pyridoxal and pyridoxal phosphate. Model systems composed of equal molar concns. of lysine with either pyridoxal or pyridoxal phosphate were used to study the effect of proton transfer on Schiff base formation. Pyridoxylidenelysine was found to be the major product in both lysine/pyridoxal and lysine/pyridoxal phosphate systems. Quantitation of residual pyridoxal and pyridoxal phosphate was conducted using an HPLC to evaluate the degradation of pyridoxal and pyridoxal phosphate. Both the free phosphate ion in the buffer system and the bound phosphate on pyridoxal phosphate can enhance the formation of the Schiff base. The phosphate group serves as both proton donor and acceptor, which catalyzes the Schiff base formation. The aldehyde group on pyridoxal phosphate was found to be much more reactive than that on pyridoxal. The bound phosphate group on pyridoxal phosphate, with proton donating and accepting groups in close proximity, can simultaneously donate and accept protons, thus enhancing Schiff base formation between the aldehyde group and the ε-amino group. The deterioration rate of pyridoxal phosphate was faster than that of pyridoxal in an aqueous system.

IT 2440-59-7
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (effect of phosphate on Schiff base formation between pyridoxal and lysine)
RN 2440-59-7 HCAPLUS
CN L-Lysine, N6-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:445765 HCAPLUS
DOCUMENT NUMBER: 133:219379
TITLE: Free energy requirement for domain movement of an enzyme
AUTHOR(S): Ishijima, Jun; Nakai, Tadashi; Kawaguchi, Shin-Ichi; Hirotsu, Ken; Kuramitsu, Seiki
CORPORATE SOURCE: Department of Biology, Graduate School of Science, Osaka University, Osaka, 560-0043, Japan
SOURCE: Journal of Biological Chemistry (2000),

Updated Search

275(25), 18939-18945
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

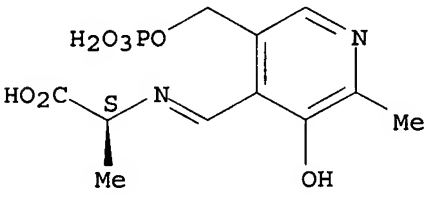
AB Domain movement is sometimes essential for substrate recognition by an enzyme. X-ray crystallog. of aminotransferase with a series of aliphatic substrates showed that the domain movement of aspartate aminotransferase was changed dramatically from an open to a closed form by the addition of only one CH2 to the side chain of the C4 substrate CH3(CH2)C(α)H(NH3+)COO-. These crystallog. results and reaction kinetics enabled us to estimate the free energy required for the domain movement.

IT 61652-32-2D, complexes with aspartate aminotransferase
RL: PRP (Properties)
(free energy requirement for domain movement of an enzyme)

RN 61652-32-2 HCAPLUS

CN L-Alanine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:261410 HCAPLUS
DOCUMENT NUMBER: 133:131624
TITLE: Quantum mechanical study of the intermediates formed following the reaction of the histidine decarboxylase's substrate and inhibitors with coenzyme
AUTHOR(S): Tahanejad, Fatemeh Sadat; Naderi-Manesh, Hossein
CORPORATE SOURCE: Department of Pharmacology, Baghiyatollah University Medical Sciences, Tehran, Iran
SOURCE: European Journal of Medicinal Chemistry (2000), 35(3), 283-289
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

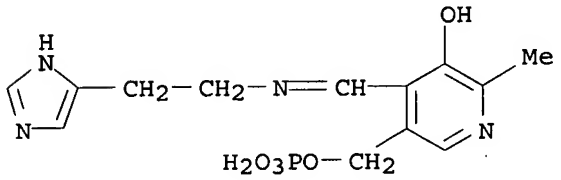
AB Histidine decarboxylase catalyzes the decarboxylation of L-histidine to histamine using pyridoxal-5'-phosphate (PLP) as coenzyme. The PM3 quantum mech. conformation method of anal. and heat of formation calcn. were carried out for intermediates which are probably formed during the interaction of histidine (substrate), (s)-α-methylhistidine, (s)-α-hydrazinohistidine, (s)-α-fluoromethylhistidine and (s)-α-difluoromethylhistidine (inhibitors) with PLP-dependent histidine decarboxylase from Morganella morganii. The results suggest that the structures of the intermediates before and after decarboxylation were found to exist in a conformation showing a planar arrangement of the

double bonds with the pyridoxylidene ring and the bond to the carboxyl group being perpendicular to this plane. After decarboxylation, all the double bonds are in the plane of the pyridoxylidene ring which facilitates the electron displacement for the following protonation at Cα. The values of the enthalpy for intermediates would increase the probability of their formation in the enzyme active site which are consistent with all available stereochem. and mechanistic data.

IT 55486-02-7
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(quantum mech. study of intermediates formed following the reaction of histidine decarboxylase substrate and inhibitors with coenzyme)

RN 55486-02-7 HCAPLUS

CN 3-Pyridinemethanol, 5-hydroxy-4-[[[2-(1H-imidazol-4-yl)ethyl]imino]methyl]-6-methyl-, α-(dihydrogen phosphate) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:301277 HCAPLUS

DOCUMENT NUMBER: 131:73929

TITLE: Spectral properties and electronic structure of pyridoxal-5'-phosphate aldimines with some amino acid phospho analogs

AUTHOR(S): Morozov, Yu. V.; Bazhulina, N. P.; Chekhov, V. O.; Bokovoy, V. A.; Osipova, T. I.; Khomutov, A. R.; Khomutov, R. M.; Khurs, E. N.

CORPORATE SOURCE: Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 117984, Russia

SOURCE: Biofizika (1998), 43(2), 196-204
CODEN: BIOFAI; ISSN: 0006-3029

PUBLISHER: Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Spectral properties, acid-base, tautomeric and conformational equilibrium for pyridoxal-5'-phosphate aldimines with phosphonous and phosphonic analogs of valine have been investigated. The spectral properties of these analogs have been shown to be close to those of pyridoxal-5'-phosphate aldimines with natural valine while their equilibrium differ drastically. The stability of bonds in the aldimine amino acid moiety, which undergo changes in the course of pyridoxal-5'-phosphate enzymic reactions, is investigated for pyridoxal-5'-phosphate aldimines with alanine and their phosphonous and phosphonic analogs. The influence of ionic state of the whole mol. and of its moieties as well as of its conformation state on the stability of bonds under discussion has been also elucidated.

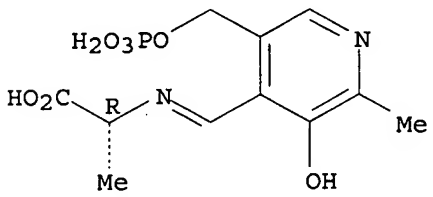
IT 125316-67-8
RL: PRP (Properties)
(spectral properties and electronic structure of pyridoxal-5'-phosphate aldimines with amino acid phospho analogs)

RN 125316-67-8 HCAPLUS

CN D-Alanine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-

pyridinyl]methylene]- (CA INDEX NAME)

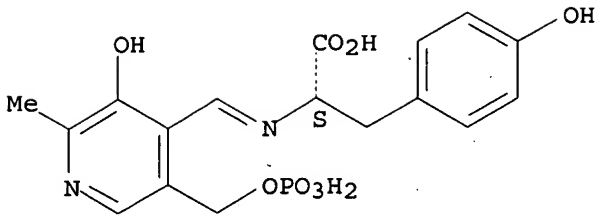
Absolute stereochemistry.
Double bond geometry unknown.



L12 ANSWER 8 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:287007 HCAPLUS
DOCUMENT NUMBER: 131:19260
TITLE: Spectral properties of pyridoxal 5'-phosphate aldimines with some aromatic amino acids and their analogs: tautomeric and isomeric equilibria
AUTHOR(S): Morozov, Yu. V.; Bazhulina, N. P.; Bokovoi, V. A.; Kuznetsova, N. V.; Kartasheva, O. N.; Osipova, T. I.; Khurs, E. N.
CORPORATE SOURCE: Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 117984, Russia
SOURCE: Bioorganicheskaya Khimiya (1998), 24(8), 631-637
CODEN: BIKHD7; ISSN: 0132-3423
PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Spectral properties of the ionic forms of pyridoxal 5'-phosphate aldimines with phenylalanine, tyrosine, phosphonic, and phosphonous phenylalanine analogs and pH-dependent transitions between these forms were studied. The tautomeric and isomeric composition of these equilibrium mixts. was determined The spectral properties of these compds. were shown to be very close to those of the aldimines of pyridoxal 5'-phosphate with the other amino acids studied previously. At the same time, significant differences in the content of the tautomeric and conformational forms were observed The substitution of the phosphonic or phosphonous group for the carboxyl group also influenced the content of various tautomeric forms, planar and rotational conformers.
IT 35314-36-4
RL: PRP (Properties)
(tautomeric and isomeric equilibrium of pyridoxal phosphate aldimines with aromatic amino acids and their analogs)
RN 35314-36-4 HCAPLUS
CN L-Tyrosine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

Updated Search



L12 ANSWER 9 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:84967 HCAPLUS
DOCUMENT NUMBER: 130:263985
TITLE: Time-resolved fluorescence of O-acetylserine sulfhydrylase
AUTHOR(S): Benci, Sara; Vaccari, Silvia; Mozzarelli, Andrea; Cook, Paul F.
CORPORATE SOURCE: Institute Physical Sciences and Istituto Nazionale per la Fisica della Materia, University Parma, Parma, 43100, Italy
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1999), 1429(2), 317-330
CODEN: BBAEDZ; ISSN: 0167-4838
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

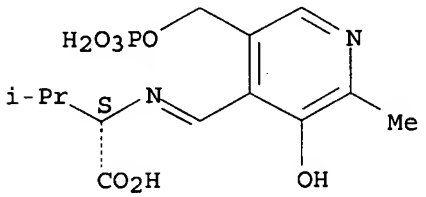
AB Static and time-resolved fluorescence of the internal aldimine of pyridoxal 5'-phosphate (PLP)-dependent O-acetylserine sulfhydrylase (I) and those of free PLP, and the PLP-L-valine Schiff base were measured to gain insight into the photophysics of PLP bound to I. Exciting at 330 nm, the free coenzyme exhibited a band at 415 nm, whereas PLP-valine and I (also when excited at their absorbance maxima) exhibited a structured emission with a peak at 420 nm and shoulders at 490 and 530 nm. The emission bands at 420 and 490 nm were attributed to the enolimine and ketoenamine tautomers of the internal aldimine, resp., whereas the 530-nm emission might arise from a dipolar species formed upon proton dissociation in the excited state. Time-resolved fluorescence of I (PLP-valine), excited at 412 nm (415 nm) and collected at λ = >470 nm, indicated the presence of 2 components characterized by lifetimes (τ) of 0.6 and 3.8 ns with equal fractional intensity (f). In the presence of acetate, the slow component dominated I emission with an f value of 0.98. Excitation at 350 nm as a function of emission wavelengths (400-560 nm) showed at least 3 components. The f value of the slow component increased from 400 to 440 nm, then decreased, whereas the f value of the intermediate and fast components behaved in the opposite way. The results indicated that: (1) the fast component was associated with the emission at 530 nm; (2) the slow component was associated with the emission at 420 nm; (3) a fast additive component, characterized by a very short lifetime, was present on the blue side of the emission spectrum; (4) the intermediate component resulted from overlapping contributions, including the emission of the band at 490 nm, that could not be resolved; (5) the increased emission at 490 nm; caused by acetate binding was likely due to the stabilization of the ketoenamine tautomer induced by an increase in the polarity of the active site microenvironment and/or a decrease in proton dissociation in the excited state; (6) excitation at 330 nm, where the enolimine tautomer absorbs, led to emission decays typical of the ketoenamine.

IT 32653-39-7
RL: PRP (Properties)
(time-resolved fluorescence of O-acetylserine sulfhydrylase, pyridoxal

Updated Search

5'-phosphate (PLP), and the PLP-valine Schiff base)
RN 32653-39-7 HCAPLUS
CN L-Valine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

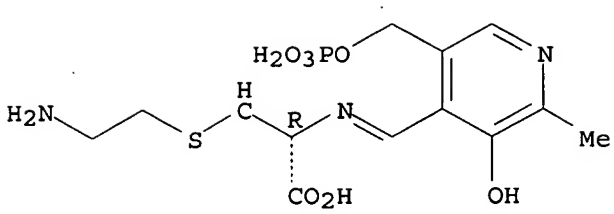


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 197 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:588431 HCAPLUS
DOCUMENT NUMBER: 129:312691
TITLE: S-Adenosylmethionine: a 'poor man's coenzyme B12' in the reaction of lysine 2,3-aminomutase
AUTHOR(S): Frey, P. A.; Ballinger, M. D.; Reed, G. H.
CORPORATE SOURCE: Institute for Enzyme Research, The Graduate School, and Department of Biochemistry, College of Agricultural and Life Science, Univ. of Wisconsin-Madison, Madison, WI, 53705, USA
SOURCE: Biochemical Society Transactions (1998), 26(3), 304-310
CODEN: BCSTB5; ISSN: 0300-5127
PUBLISHER: Portland Press Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Adenosylcobalamin has long been recognized as the coenzyme for enzymes that catalyze intramol. rearrangements in which an unactivated, carbon-bound hydrogen atom undergoes a 1,2-migration, concomitant with the counter migration of a functional group or a carbon fragment. An exception is the reaction of lysine 2,3-aminomutase from Clostridia which does not require coenzyme B12. S-adenosylmethionine (SAM) and an iron-sulfur center function in place of adenosylcobalamine. The coenzymes of lysine 2,3-aminomutase, SAM, pyridoxal-5'-phosphate (PLP) and an iron-sulfur center are well known for their classical roles in biol. methylation, metabolism of amino acids, and biol. electron transfer, resp. However, their functions in the conversion of lysine into β-lysine are mechanistically novel.
IT 214678-15-6
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(S-Adenosylmethionine in reaction of lysine 2,3-aminomutase)
RN 214678-15-6 HCAPLUS
CN Ethyl, 1-[(2-aminoethyl)thio]-2-carboxy-2-[[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene]amino]-, conjugate monoacid, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

Updated Search



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECO

Updated Search